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Factor analysis in IR spectroscopic studies of hydrogen bondings and conformations

Remizov A., Skochilov R.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

Within the frames of the factor analysis a new approach to extract spectra of components from spectra of solutions was developed. This allows one to determine concentrations of components without using a priori information. By this method, the IR spectra of tert-butyl hydroperoxide (TBH) in various solvents were investigated. In these solutions there are gauche and trans conformations of monomers of TBH and self-associations of TBH (dimers and trimers) are analyzed. The spectra of components and their concentrations are determined. Equilibrium constants of dimerization and trimerization and thermodynamic parameters of complexes are found. The factor analysis has been used in the spectroscopic study of trans and gauche conformations of 1,2-di-(p-nitrophenyl)ethane in acetone. The enthalpy and entropy differences of the trans and gauche conformations have been determined.

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Keywords

Concentrations of components of a mixture, Factor analysis, Infrared spectra, Spectra of components